The modified XXZ Heisenberg chain, conformal invariance, surface exponents of c < 1 systems, and hidden symmetries of the finite chains *

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Abstract: The spin-1/2 XXZ Heisenberg chain with two types of boundary terms is considered. For the first type, the Hamiltonian is hermitian but not for the second type which includes the $U_q[SU(2)]$ symmetric case. It is shown that for a certain "tuning" between the anisotropy angle and the boundary terms the spectra present unexpected degeneracies. These degeneracies are related to the structure of the irreducible representations of the Virasoro algebras for c < 1.

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Some time ago [1] we have addressed ourselves the problem of universality classes in the case of two-dimensional systems at a second-order phase transition. Assuming that conformal invariance can be used (which is not always the case), one is tempted to define the universality class through a certain modular invariant partition function corresponding to a given central charge of the Virasoro algebra. In the case of the minimal series for example, the modular invariant partition functions were given by Cappelli et al. [2]. A modular invariant partition function does not however specify "who is who" in the list of primary fields. A given primary operator however can be associated with a symmetry breaking operator (corresponding to an order parameter) or to a thermal operator (its anomalous dimension determines the specific heat). Phrased in a different way, the question is if two ore more systems defined on a lattice and having different symmetries cannot correspond to the same modular invariant partition function. We think that the answer is "yes" and that the complete description of the system needs the knowledge of all the partition functions corresponding to the different boundary conditions (BC) compatible with translational invariance (all toroidal BC). In order to get an insight into the problem we have shown that one can project out from the Coulomb gas partition functions, the partition functions of several systems, all of them having the same modular invariant partition function. In this way, for the minimal series we have shown that for each given modular invariant partition function we have four different systems and we called the corresponding series the p-state Potts, tricritical p-state Potts, the O(p), and the low temperature O(p) models. A similar picture was proposed earlier on quite different grounds by Nienhuis et al. [3]. Behind each of the series stay different short-distance algebras. This work was extended later [4] to the case of the N=1 superconformal series where for each for each of the modular invariant partition functions of Cappelli [5] we have found two different models. One remarkable fact is that when applied to the XXZ spin-1/2 Heisenberg chain, for one class of models, the projection mechanism also works for finite chains. A similar phenomenon occurs if the projection mechanism is applied to the Fateev-Zamolodchikov spin-1 quantum chain [4].

In the present lecture we will describe the partition functions of the minimal models described above in the case of *free BC*. As a by-product we will show some "miraculous" properties of the XXZ chain with modified BC. Some of the results presented here were already published [6], some others are new

The modified XXZ model with N sites is defined by the Hamiltonian

$$H = -\frac{\gamma}{2\pi \sin \gamma} \left\{ \sum_{j=1}^{N-1} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y - \cos \gamma \sigma_j^z \sigma_{j+1}^z \right] + p \sigma_1^z + p' \sigma_N^z \right\} , \tag{1}$$

where σ^x , σ^y , and σ^z are Pauli matrices and p, p' describe the coupling to external fields. The special case p = p' = 0 corresponds to free BC.

Instead of describing the anisotropy of the Hamiltonian through the parameter γ it is useful to define

$$h = \frac{1}{4} \left(1 - \frac{\gamma}{\pi} \right)^{-1} \left(h \ge \frac{1}{4} \right) . \tag{2}$$

As discussed in Ref. [7], h is related to the compactification radius R of the bosonic string $(h=R^2/2)$. It also is convenient to denote

$$p = i \sin \gamma \coth \alpha$$
 , $p' = i \sin \gamma \coth \alpha'$, (3)

where α and α' are complex parameters. It turns out that two parametrisations of α and α' leave the spectrum real:

$$\alpha = -\frac{i\pi}{2}\psi + \frac{i\pi}{2}a \quad , \quad \alpha' = -\frac{i\pi}{2}\psi - \frac{i\pi}{2}a \tag{4.a}$$

where ψ and a are real (in this case the Hamiltonian is hermitian), and

$$\alpha = -\frac{i\pi}{2}\psi + \frac{\pi}{2}b$$
 , $\alpha' = -\frac{i\pi}{2}\psi - \frac{\pi}{2}b$ (4.b)

where ψ and b are real (in this case the Hamiltonian is *not* hermitian). Note that for $a=b=0, \psi=1$ one recovers the case of free BC and that the two BC coincide for a=b=0. The case $b\to\infty$ for the BC (4.b) is very special since in this case the Hamiltonian has the quantum algebra $U_q[SU(2)]$ with $q=e^{i\gamma}$ as symmetry.

We notice that the charge operator

$$\hat{Q} = \frac{1}{2} \sum_{j=1}^{N} \sigma_j^z \tag{5}$$

commutes with H and that its eigenvalues Q are integer (half-integer) when N is even (odd). Let $E_{Q;i}(N)$ be the energy levels, $i=0,1,\ldots$, in the charge sector Q of the Hamiltonian with N sites and $E_0^F(N)$ the ground-state energy of the Hamiltonian with free BC. We consider the following quantities:

$$\overline{E}_{Q;i} = \frac{N}{\pi} \left(E_{Q;i}(N) - E_0^F(N) \right)$$

$$\mathcal{E}_Q(N,z) = \sum_i z^{\overline{E}_{Q;i}(N)}$$

$$\mathcal{E}_Q(z) = \lim_{z \to \infty} \mathcal{E}_Q(N,z) .$$
(6)

Using numerical estimates from chains up to 18 sites as well as analytical methods [8] , we have obtained the following ansatz:

$$\mathcal{E}_{Q}(z) = z^{\frac{(Q+\varphi)^{2}}{4h}} \Pi_{V}(z) \quad , \quad \Pi_{V}(z) = \prod_{m=1}^{\infty} (1-z^{m})^{-1} \quad , \tag{7}$$

where $\varphi = 2h(1 - \psi)$ independent of a or b (see Eqs. (4.a,4.b)). Notice that $\mathcal{E}_Q \neq \mathcal{E}_{-Q}$. In the $U_q[SU(2)]$ symmetric case the partition functions are very different, one obtains [9]:

$$\mathcal{E}_{Q} = \mathcal{E}_{-Q} = \sum_{j=|Q|}^{\infty} \left[z^{\frac{(2j+1-h)^{2}}{4h}} - z^{\frac{(2j+1+h)^{2}}{4h}} \right] \Pi_{V}(z) . \tag{8}$$

In the expressions (7) and (8), Q is an integer or half-integer. This result is very interesting because from Eq. (7) we learn that the operator content in the charge sector Q is given by a single irrep of a shifted U(1) Kac-Moody algebra [7], the shift φ being related to ψ . The expression (7) is the starting point of the Feigin-Fuchs construction [10, 11] of irreps of Virasoro algebras with c<1 starting from irreps with c=1 (this is the central charge of the XXZ chain). This construction will allow us to identify the operator content of systems with c<1 with free, fixed, and mixed BC. First, we recall that for c<1 the central charge is quantized:

$$c = 1 - \frac{6}{m(m+1)}$$
 $(m = 3, 4, ...)$, (9)

and for a given m, the highest weights $\Delta_{r,s}$ of unitary irreps are

$$\Delta_{r,s} = \frac{[(m+1)r - ms]^2 - 1}{4m(m+1)} \quad , \quad 1 \le r \le m-1 \quad , \quad 1 \le s \le m \quad . \tag{10}$$

The corresponding character functions are:

$$\chi_{r,s} = \Omega_{r,s} - \Omega_{r,-s}$$

$$\Omega_{r,s} = \sum_{\alpha = -\infty}^{\infty} z^{\frac{[2m(m+1)\alpha + (m+1)r - ms]^2 - 1}{4m(m+1)}} \Pi_V(z) .$$
(11)

In order to apply the Feigin-Fuchs procedure, let us assume that we have fixed h and φ . Instead of considering $E_0^F(N)$ as ground-state energy, we take as ground-state energy $E_{0;0}(N)$, i.e. the ground-state in the charge-zero sector of the Hamiltonian (1) with γ , p and p' fixed. Next, instead of considering charges taking values in \mathbb{Z} or $\mathbb{Z}+1/2$, it is convenient to work with charges in \mathbb{Z}_n or $\mathbb{Z}_{n+1/2}$, respectively (the values of n will be fixed later). Thus, instead of Eqs. (6) and (7) we have

$$\overline{F}_{\overline{q};i} = \frac{N}{\pi} \left(E_{\overline{q};i} - E_{0;0}(N) \right)$$

$$\mathcal{F}_{\overline{q}}(N,z) = \sum_{i} z^{\overline{F}_{\overline{q};i}}$$

$$\mathcal{F}_{\overline{q}}(z) = \lim_{N \to \infty} \mathcal{F}_{\overline{q}}(N,z) = \sum_{\alpha = -\infty}^{\infty} z^{\frac{(n\alpha + \overline{q} + \varphi)^{2} - \varphi^{2}}{4h}} \Pi_{V}(z) ,$$
(12)

where $\overline{q} = 0, 1, \dots, n-1$ for N even and $\overline{q} = \frac{1}{2}, \frac{3}{2}, \dots, n-\frac{1}{2}$ for N odd. We now choose

$$h = \frac{n^2}{4m(m+1)}$$
 , $\varphi = \frac{n}{2m(m+1)}$, (13)

that is $\psi = 1 - 1/n$, and get

$$\mathcal{F}_{\overline{q}}(z) = \sum_{\alpha = -\infty}^{\infty} z^{\frac{[2m(m+1)\alpha + 2m(m+1)\overline{q}/n + 1]^2 - 1}{4m(m+1)}} \Pi_V(z) . \tag{14}$$

Since the finite-size scaling spectrum given by Eq. (7) stays positive for any positive h, we will assume that we can use the equations above for $0 < h < \frac{1}{4}$ also (see Eq. (2)). The four choices of n given in Table 1 divide the domain $h \ge \frac{1}{6}$ into four regions which correspond to the p-state Potts models, tricritical p-state Potts models, O(p) models, and low temperature O(p) models [12]. Let us first consider the case of the p-state Potts model (n=m+1). Comparing Eqs. (11) and (14), we have

$$\mathcal{F}_{-\overline{q}} = \Omega_{1,2\overline{q}+1} \tag{15}$$

and

$$\chi_{1,2v+1} = \mathcal{F}_{-v} - \mathcal{F}_{v+1} \qquad \overline{q} \text{ integer}$$
(16)

$$\chi_{1,2v} = \mathcal{F}_{\frac{1}{2}-v} - \mathcal{F}_{\frac{1}{2}+v} \qquad \overline{q} \text{ half-integer} .$$
(17)

In order to clarify the physical significance of our results, let us take m=3, n=4. We find

$$\chi_{1,1} = \mathcal{F}_0 - \mathcal{F}_1 \quad , \quad \Delta = 0 \quad ,$$

$$\chi_{1,3} = \mathcal{F}_{-1} - \mathcal{F}_2 \quad , \quad \Delta = \frac{1}{2} \quad .$$
(18)

These are precisely the surface exponents of the Ising model (or, alternatively, the exponents for fixed BC which are the same) [13, 14]. If we take \overline{q} half-integer, we have

$$\chi_{1,2} = \mathcal{F}_{-\frac{1}{2}} - \mathcal{F}_{\frac{3}{2}} , \quad \Delta = \frac{1}{16} ,$$
(19)

Table 1: Definition of the models. The arguments of the cosine functions are taken positive. The values of n occur in Eq. (13).

	p-state Potts 0	Tricritical p -state Potts 0
Definition of the model	$\frac{1}{2}\sqrt{p} = \cos\pi(1 - \frac{1}{4h})$	$\frac{1}{2}\sqrt{p} = \cos\pi(\frac{1}{4h} - 1)$
Domain of h	$\frac{1}{2} \ge h \ge \frac{1}{4}$	$\frac{1}{4} \ge h \ge \frac{1}{6}$
Values of n	m+1	m

	$O(p) \\ -2$	Low temperature $O(p)$ -2
Definition of the model	$\frac{1}{2}p = \cos \pi (\frac{1}{h} - 1)$	$\frac{1}{2}p = \cos \pi (1 - \frac{1}{h})$
Domain of h	$1 \ge h \ge \frac{1}{2}$	$h \ge 1$
Values of n	2m	2(m+1)

which corresponds to the case of mixed BC [13] . We now consider m=5, n=6 (the three-state Potts model) and \overline{q} integer. We obtain

$$\chi_{1,1} = \mathcal{F}_0 - \mathcal{F}_1 \quad , \quad \Delta = 0 \quad ,$$

$$\chi_{1,3} = \mathcal{F}_{-1} - \mathcal{F}_2 \quad , \quad \Delta = \frac{2}{3} \quad ,$$

$$\chi_{1,5} = \mathcal{F}_{-2} - \mathcal{F}_3 \quad , \quad \Delta = 3 \quad .$$
(20)

These are again the known surface exponents (free BC) or the exponents corresponding to fixed BC. If we take \overline{q} half-integer we find

$$\chi_{1,2} = \mathcal{F}_{-\frac{1}{2}} - \mathcal{F}_{\frac{3}{2}} , \quad \Delta = \frac{1}{8} ,$$

$$\chi_{1,4} = \mathcal{F}_{-\frac{3}{2}} - \mathcal{F}_{\frac{5}{2}} , \quad \Delta = \frac{13}{8} .$$
(21)

The values $\Delta = \frac{1}{8}$ and $\Delta = \frac{13}{8}$ are indeed the exponents of the three-state Potts model with mixed BC [13]. The case m=4 does not correspond to the tricritical Ising model. It has the same modular invariant partition function as the tricritical Ising model but with another distribution of the primary fields between the charge sectors [1].

From the above considerations, we will assume that for all values of m, Eq. (16) gives us the surface (or fixed BC) exponents and Eq. (17) the exponents for mixed BC. The operator contents for free (fixed) and mixed BC for various models are given in Table 2. Let us derive some known

Table 2: The operator content for free (fixed) and mixed boundary conditions and their relation to the XXZ chain for various models. (For the p-state Potts case see Eqs. (16) and (17)).

	p-state Potts	Tricritical p -state Potts	
	$\mathcal{F}_{-\overline{q}} = \Omega_{1,2\overline{q}+1}$	$\mathcal{F}_{\overline{q}} = \Omega_{2\overline{q}+1,1}$	
Free (fixed) BC	$\chi_{1,2v+1} = \mathcal{F}_{-v} - \mathcal{F}_{v+1}$	$\chi_{2v+1,1} = \mathcal{F}_v - \mathcal{F}_{-v-1}$	
Mixed BC	$\chi_{1,2v} = \mathcal{F}_{-v + \frac{1}{2}} - \mathcal{F}_{v + \frac{1}{2}}$	$\chi_{2v,1} = \mathcal{F}_{v-\frac{1}{2}} - \mathcal{F}_{-v-\frac{1}{2}}$	

	O(p)	Low temperature $O(p)$
	$\mathcal{F}_{\overline{q}} = \Omega_{\overline{q}+1,1}$	$\mathcal{F}_{-\overline{q}} = \Omega_{1,\overline{q}+1}$
Free (fixed) BC	$\chi_{r,1} = \mathcal{F}_{r-1} - \mathcal{F}_{-r-1}$	$\chi_{1,s} = \mathcal{F}_{1-s} - \mathcal{F}_{1+s}$
Mixed BC	m odd only $\chi_{r,\frac{m-1}{2}} = \mathcal{F}_{\frac{m}{2}-1-r} - \mathcal{F}_{\frac{m}{2}-1+r}$	m even only $\chi_{\frac{m}{2}-1,s}=\mathcal{F}_{s-\frac{m-1}{2}}-\mathcal{F}_{-s-\frac{m-1}{2}}$

results. For the tricritical Ising model (m=n=4), we get

free BC
$$(0) \oplus \left(\frac{3}{2}\right)$$
 (22)

mixed BC
$$\left(\frac{7}{16}\right)$$
 . (23)

Equation (22) is in agreement with the result of Cardy [13], Eq. (23) is new. In the case of the O(p) models, the leading surface exponent is $\Delta_{2,1}$, again in agreement with Cardy [15].

Let us proceed with the discussion of our results by means of an example. From the first line of Eq. (20) we see that combining the finite-size scaling spectra of the $\overline{q}=0$ and $\overline{q}=1$ sectors (see Eq. (12), disregarding all the doublets (levels which occur in the sectors $\overline{q}=0$ and $\overline{q}=1$), and keeping only the singlets (levels which occur in the $\overline{q}=0$ sector only), we obtain the vacuum sector of the three-state Potts model. This is the general structure of the projection mechanism of the finite-size scaling spectra for c < 1 from the spectra for c = 1. We can go one step further and check whether the same projection mechanism also works for a *finite number of sites*. For the example of Eq. (20) this would imply that all the levels of the sector $\overline{q} = 1$ are exactly degenerate with levels of the sector $\overline{q}=0$ even for a finite number of sites, and the remaining levels in the sector $\overline{q}=0$ define the spectrum of the vacuum sector of the three-state Potts model. The same picture should be valid for the $\overline{q} = -1$ and $\overline{q} = 2$ sectors as well as for the $\overline{q} = -2$ and $\overline{q} = 3$ sectors. In Table 3 we give

Table 3: Table of $\overline{F}_{\overline{q};i}(N)$ values (see Eq. (12)) for N=4, $h=\frac{3}{10}$, $\psi=\frac{5}{6}$, and several values of a and b (see Eqs. (4.a) and (4.b) . The underlined levels occur in the three-state Potts model with free BC. (The XXZ chain with 2N sites gives the p-state Potts model with N sites and free BC.)

$a=\frac{2}{3}$		$a = \frac{1}{6}$		a=b=0	
$\overline{q} = 0$	$\overline{q} = 1$	$\overline{q} = 0$	$\overline{q} = 1$	$\overline{q} = 0$	$\overline{q} = 1$
0.000000		0.000000		0.000000	
0.869482	0.869482	0.573943	0.573943	0.566777	0.566777
1.347175	1.347175	1.128282	1.128282	1.124431	1.124431
1.407619		1.407619		1.407619	
2.022885	2.022885	1.693423	1.693423	1.689669	1.689669
2.520290	2.520290	1.992459	1.992459	1.980841	1.980841
$\overline{q} = -1$	$\overline{q} = 2$	$\overline{q} = -1$	$\overline{q} = 2$	$\overline{q} = -1$	$\overline{q} = 2$
0.471151		0.471151		0.471151	
1.071362		1.071362		1.071362	
1.671573		1.671573		1.671573	
2.386227	2.386227	1.928985	1.928985	1.920189	1.920189
$\overline{q} = -2$	$\overline{q} = 3$	$\overline{q} = -2$	$\overline{q} = 3$	$\overline{q} = -2$	$\overline{q} = 3$
1.806467		1.806467		1.806467	

b=1		b=2		$b\!=\!\infty$	
$\overline{q} = 0$	$\overline{q} = 1$	$\overline{q} = 0$	$\overline{q} = 1$	$\overline{q} = 0$	$\overline{q} = 1$
0.000 000		0.000000		0.000000	
0.485791	0.485791	0.471833	0.471833	0.471151	0.471151
1.079782	1.079782	1.071757	1.071757	1.071362	1.071362
1.407619		1.407619		1.407619	
1.668001	1.668001	1.671294	1.671294	1.671573	1.671573
1.838081	1.838081	1.808041	1.808041	1.806467	1.806467
$\overline{q} = -1$	$\overline{q} = 2$	$\overline{q} = -1$	$\overline{q} = 2$	$\overline{q} = -1$	$\overline{q} = 2$
0.471151		0.471151		0.471151	
1.071362		1.071362		1.071362	
1.671573		1.671573		1.671573	
1.823501	1.823501	1.807257	1.807257	1.806467	1.806467
$\overline{q} = -2$	$\overline{q} = 3$	$\overline{q} = -2$	$\overline{q} = 3$	$\overline{q} = -2$	$\overline{q} = 3$
1.806467		1.806467		1.806467	

the values of $\overline{F}_{\overline{q};i}$ for four sites $(h=\frac{3}{10}\ ,\ \psi=\frac{5}{6})$, and $a=\frac{2}{3},\ a=\frac{1}{6},\ a=b=0,\ b=1,2,$ and ∞ . The case $b=\infty$ corresponds to the $U_q[SU(2)]$ symmetric case with $q=\exp(\frac{i\pi}{6})$. Leaving aside for the moment the case $b=\infty$, we notice the following features:

- 1. The spectra have doublets and singlets. This suggests a supplementary symmetry in the Hamiltonian. This symmetry goes away if h and φ are not "tuned" like in Eq. (13) $(\psi = 1 \frac{\gamma}{\pi})$.
- 2. The doublets occur (like in Table 3 in the sectors \mathcal{F}_0 and \mathcal{F}_1 for example) in order to allow the projection mechanism to occur, but also between other sectors (this can be seen for a larger number of sites).
- 3. The doublets "move" if we modify the values of the parameters a and b (like in Table 3) or do not (as one can notice for a larger number of sites).
- 4. For larger number of sites (eight for the example presented in Table 3), the degeneracy of a level can be larger than two, the levels are however distributed among the various sectors such that the projection mechanism works.
- 5. The projection mechanism works even for a finite number of sites! The levels left (the singlets) after projecting out the doublets occurring in the corresponding charge sectors give precisely the spectrum of the three-state Potts model with free (fixed) BC (see Table 2 of Ref. [15]).

We now consider the $U_q[SU(2)]$ symmetric case $b=\infty$. In this case the multiplets are much larger. Since $q = \exp(\frac{i\pi}{6})$, the multiplets are (2j+1)-dimensional with j=0,1,2 for \overline{q} even and $j=\frac{1}{2},\frac{3}{2}$ for \overline{q} odd. The projection mechanism is very different in this case (see Ref. [9], where a superb explanation of the projection mechanism is given). One again obtains the exponents (20) but with different multiplicities: (0) and (3) occur once, but $\left(\frac{2}{3}\right)$ occurs twice.

The same pattern occurs for an odd number of sites and for any value of m as long as n=m+1. The projection mechanism does *not* work however for the O(p) (n=2m) or low temperature O(p) (n=2(m+1)) models where one does not observe the required doublets in the spectra. The existence of multiplets for $\psi=1-\frac{\gamma}{\pi}$ suggesting a discrete non-local symmetry is one of the big mysteries of our work.

The projection mechanism described above can certainly be extended to other systems since the structure of the character expressions of extended algebras is always similar to Eq. (11). The first step in this direction in order to derive the surface exponents of the N=1 superconformal model was already made [16].

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